86. (New) The computer implemented method of claim 84, wherein the spectral data comprises ^{1}H, ^{13}C, ^{15}N, ^{17}O, ^{19}F, ^{31}P or ^{35}S NMR data.

87. (New) The method of claim 86, wherein the spectral data is calculated.

88. (New) The computer implemented method of claim 82, wherein the spectral data of the test compound and the spectral data of the training set of compounds comprise ^{13}C NMR data and segmenting into bins comprises dividing the ^{13}C NMR data into sub-spectral units having a width from 0.5 ppm to 5.0 ppm.

89. (New) The computer implemented method of claim 88, wherein the ^{13}C NMR data comprises calculated ^{13}C NMR data.

90. (New) A computer readable medium having stored thereon instructions for performing the actions of claim 82.--

End

REMARKS

Status of the Application

Claims 1-26, 55-58 and 65 are currently pending and stand rejected. Claims 27-54 and 59-64 are currently withdrawn from consideration and are deleted by this Amendment.

Support for Amendments to Claims 1-3, 7, 9-15, 17-24, 55-58 and 65

Claim 1 has been amended for clarity, and support for the amendments to claim 1 may be found throughout the application, for example, at page 10, lines 11-13.

Claims 2 and 3 have been amended to correct punctuation issues.

Support for the amendments to claims 4 and 5 may, for example, be found at page 10, lines 10-11 and page 17, lines 12-16.

Claim 7 has been amended for clarity.

Claim 9 has been amended for clarity.

Support for the amendments to claim 10 may be found at page 11, lines 11-14 and page 12, lines 2-6.

Claims 11-13 have been amended for clarity.

Support for amendments to claim 14 may be found at page 66, lines 13-23.

Claim 15 has been amended for clarity.

Support for claim 17 may be found at page 66, lines 13-14 and from page 66, line 24 to page 67, line 3.

Support for the amendments to claim 18 may be found throughout the specification. Specifically, support may be found at page 9, lines 13-16; page 10, lines 10-13; page 11, lines 3-4; and in Example 7 from page 57, line 24 to page 58, line 2.

Support for amendments to claim 19 may be found at page 66, lines 13-14.

Claim 20 has been amended for clarity, but support also may be found at page 17, lines 12-13.

Claim 21 has been amended for clarity and to correct a typographical error.

Support for amendments to claim 22 may be found from page 10, line 25 to page 11 line 2.

Support for amendments to claim 23 may be found from page 10, line 25 to page 11, line 2, and at page 17, lines 12-13.

Claim 24 has been amended for clarity.

Claims 55-58 have been amended for clarity.

Support for amendments to claim 65 may be found at page 29, lines 27 - 29 and page 59, lines 3-8.

Support for new claims 66-90.

Support for new claim 66 may be found at page 62, lines 28-29.

Support for new claim 67 may be found at page 21, lines 10-20.

Support for new claim 68 may be found at page 62, lines 28-29.

Support for new claim 69 may be found throughout the specification, but more specifically, support may be found from page 9, line 1 to page 10, line 19 and at page 13, lines 5-15.

Support for new claim 70 may be found at page 10, lines 13-14.

Support for new claims 71 and 72 may be found at page 10, lines 18-19.

Support for new claim 73 may be found at page 65, lines 23-24.

Support for new claim 74 may be found at page 10, lines 25-29.

Support for new claim 75 may be found at page 10, lines 3-9; page 12, lines 11-14; and at page 21, lines 26-28.

Support for new claim 76 may be found at page 10, line 4.

Support for new claim 77 may be found at page 21, lines 13-14 and page 63, lines 3-10.

Support for new claims 78 and 79 may be found at page 10, lines 3-9 and page 12, lines 11-14.

Support for new claim 80 may be found at page 27, lines 23-24 and page 66, lines 13-23.

Support for new claim 81 may be found at page 34, line 25.

Support for new claim 82 may be found throughout the specification, but more specifically, from page 10, line 20 to page 11, line 18, and from page 25, line 8 to page 29, line 2. Examples 1 through 4 are particular embodiments of such a method.

Support for new claim 83 may be found at page 10, lines 25-28.

Support for new claim 84 may be found at page 12, lines 11-14.

Support for new claim 85 may be found at page 65, lines 4-7.

Support for new claim 86 may be found at page 62, lines 28-29.

Support for new claim 87 may be found at page 21, lines 10-20.

Support for new claim 88 may be found at page 34, line 25.

Support for new claim 89 may be found at page 21, lines 13-14 and page 63, lines 3-10.

Support for new claim 90, may be found at page 14, lines 2-4.

Objections to the Specification

The disclosure was objected to for containing embedded hyperlinks and/or other forms of browser-executable codes, and for failing to have a period after the number in claim 3. Applicants have deleted the embedded hyperlinks and other forms of browser-executable codes from the disclosure.

Applicants have added a period to Claim 3 by this Amendment.

In view of the requested specification amendments, applicants respectfully request that the objections to the specification be withdrawn.

Rejections under 35 U.S.C. § 112, First Paragraph.

Claim 65 was rejected as allegedly containing subject matter which was not described in the specification in such a way as to reasonably convey to one skilled in the relevant art that the inventors, at the time of the application was filed, had possession of the claimed invention. Applicants traverse this rejection and ask that it be withdrawn.

Predicting whether a test compound possesses at least one of various biological, chemical and physical endpoints is amply supported throughout the application as filed. For example, on page 29, lines 27 - 29 the application states that "[o]nce spectral data are gathered for a set of compounds, an SDAR may be generated with reference to a multitude of biological, chemical, or physical endpoints for which data is available." On page 59, lines 3-8 the application states that "[m]ultiple endpoints may be utilized to establish multiple SDARs from a single set of spectral data." Further it states "[c]ompounds then may be screened based upon their spectra using multiple SDARs for any combination of desirable or undesirable activities." These statements clearly show that applicants were in possession of the subject matter of claim 65 at the time of the application.

Claim 65 has nonetheless been amended to address the allegation (discussed below) that claim 65 "is confusing because it adds steps with respect to predicting physical and chemical properties that no longer correspond to the goal of the preamble of the claim [1]."

Rejections under 35 U.S.C. § 112, Second Paragraph

Claims 1-26, 55-58 and 65 were rejected under 35 U.S.C. § 112, second paragraph for allegedly being indefinite for failing to particularly point out and distinctly claim the subject matter which applicants regard as their invention. Applicants traverse this rejection and ask that it be withdrawn.

In particular, claim 1 was rejected for allegedly being confusing in reciting the phrase "derived not exclusively from the assigned spectral data," and for alleged inconsistencies. Applicants disagree and respectfully request that the rejection be withdrawn. The term "assigned spectral data" would be understood by one of ordinary skill in the art to mean spectral data that has not been correlated to particular structural features of the training set compounds. Both "assigned" and "unassigned" spectral data may be obtained for training set compounds and used to derive a pattern according to the claimed method. However, as discussed throughout the

specification, an advantage of the disclosed SDAR methods is that the spectral data need not be "assigned" to their underlying structural features to serve as descriptors. In contrast, many prior art methods of using spectral data as descriptors can use only "assigned" spectral data (see, for example, the Background discussion from page 5, line 15 to page 6, line 8).

Claim 1 has nonetheless been amended to present the subject matter in an alternative manner. As amended, claim 1 now clarifies that a pattern of spectral data associated with the biological activity is derived from spectral data of a training set of compounds with known biological activities, and that similarities are detected between the pattern associated with the biological activity and a pattern of spectral data for the test compound to determine whether the test compound is predicted to share the biological activity. Amended claim 1 emphasizes that it is the pattern of spectral data derived from the training set data, and not the training set spectral data itself, that is compared to the test compound's spectral data. In view of the requested amendments, applicants respectfully request that the rejection of Claim 1 under 35 U.S.C. § 112, second paragraph be withdrawn.

Claim 7 was rejected as allegedly being confusing in its dependency on claim 6. Applicants disagree, but have amended claim 7 solely for clarity. Claim 7 is not confusing and further limits claim 6. Applicants therefore request that the rejection of claim 7 under 35 U.S.C. §112, second paragraph be withdrawn.

The Office action alleges that computer implementation is implicit to the disclosed method of claim 1. Applicants disagree with this allegation. Although it may be desirable to use a computer, a person of ordinary skill in the art could manually perform calculations that yield a pattern from spectral data. Such a manually derived pattern could also be compared, with or without computer implementation, to the spectral data of a test compound to make a qualitative prediction of whether the test compound possesses a particular biological activity (or chemical or physical activity). For example, as demonstrated in the specification at page 28, lines 7-28, it is possible to visually make a qualitative prediction from a canonical variate plot.

Claim 14 was rejected under 35 U.S.C. § 112, second paragraph for allegedly failing to further limit the subject matter of claim 1. Applicants traverse this rejection and ask that it be withdrawn. Claim 14 has been rewritten to recite the phrase "wherein detecting similarities between the pattern of spectral data associated with the biological activity of the training set and the pattern of spectral data for the test compound comprises statistical pattern recognition."

Claim 14 further limits the subject matter of claim 1, since as taught in the specification there are a number of methods of detecting and comparing patterns, including statistical methods and artificial intelligence methods. Applicants therefore request that the rejection of claim 14 under 35 U.S.C. §112, second paragraph be withdrawn.

Claim 17 was rejected under 35 U.S.C. § 112, second paragraph for allegedly failing to further limit the subject matter of claim 1. Applicants traverse this rejection and request that it be withdrawn. Claim 17 has been rewritten to recite "wherein detecting similarities between the pattern of spectral data associated with the biological activity of the training set and the pattern of spectral data for the test compound comprises artificial intelligence pattern recognition." Claim 17 further limits the subject matter of claim 1, since as taught in the specification there are a number of methods of detecting and comparing patterns, including statistical methods and artificial intelligence methods. Applicants therefore request that the rejection of claim 17 under 35 U.S.C. §112, second paragraph be withdrawn.

Claim 18 was rejected under 35 U.S.C. §112, second paragraph for allegedly appearing to be a method rather than the recited "system," and for allegedly not including a step of predicting a biological activity as indicated in the preamble. Applicants traverse the rejection and ask that it be withdrawn. Claim 18 has been rewritten as a method claim and now recites "predicting the biological activity of the test compound by comparing the pattern of spectral data associated with the biological activity to the spectral data of the test compound to determine whether the spectral data of the test compound is similar to the spectral pattern associated with the biological activity of the training set and the test compound is predicted to share the biological activity." As such, the rejection of claim 18 under 35 U.S.C. §112, second paragraph should be withdrawn, and applicants request such action.

Claim 56 was rejected under 35 U.S.C. §112, second paragraph for allegedly being confusing and failing to limit the subject matter of claim 21. Applicants traverse this rejection and ask that it be withdrawn. Claim 56 has been rewritten to depend from claim 18, and now recites "[t]he computer implemented method of claim 18, wherein the spectral data comprises calculated spectral data." Since claim 56 now recites only calculated spectral data, it clearly limits the subject matter of claim 18 and is not confusing. Applicants request that the rejection of claim 56 under 35 U.S.C. §112, second paragraph be withdrawn.

Claim 65 was rejected under 35 U.S.C. §112, second paragraph for allegedly adding steps that did not correspond to the preamble goal. Applicants traverse this rejection and ask that it be withdrawn. Claim 65 has been rewritten to recite "predicting a second biological activity of the test compound by comparing the spectral data of the test compound to a second pattern of spectral data associated with a second biological activity to determine if the test compound shares the second biological activity, the second pattern derived using the scaled spectral data and known endpoints of the training set of compounds for the second biological activity." This recitation clearly falls within the preamble goal, and emphasizes that the disclosed methods may be used to determine whether a compound possesses any number of properties (as was discussed previously with regard to the rejection of claim 65 under 35 U.S.C. §112, first paragraph). Applicants therefore request the rejection of claim 65 under 35 U.S.C. §112, second paragraph be withdrawn.

Rejections under 35 U.S.C. §102(a)

1. Beger et al.

Claims 18-19, 21, 26 and 56-58 were rejected as allegedly being anticipated by Beger et al. ("Development of ^{13}C NMR and Mass Spectra-based Structure-Activity Relationships for Estrogenictiy," 1998 FDA Science Forum, "Biotechnology: Advances, Applications and Regulatory Challenges," Washington D.C., December 8-9, 1998). Applicants traverse this rejection and ask that it be withdrawn.

As amended, claim 18 includes, amongst other features, the feature of scaling spectral data. As correctly noted in the Office action, scaling spectral data is not taught or suggested by Beger et al. Beger et al. shows only that spectral data may be clustered by cluster analysis. Cluster analysis identifies features shared by groups of compounds, and does not include scaling. Therefore, claim 18 is not anticipated by Beger et al. Applicants respectfully request that the rejection of claim 18 under 35 U.S.C. § 102(a) be withdrawn.

Claims 19, 21 and 26 are not anticipated by Beger et al. for at least the reasons given for claim 18. Applicants request that the rejection of claims 19, 21 and 26 under 35 U.S.C. § 102(a) be withdrawn.

Claim 56 is not anticipated by Beger et al. for at least the reasons given for claim 18. In addition, Beger et al. does not teach or suggest calculated spectral data as recited in claim 56. Applicants request that the rejection of claim 56 under 35 U.S.C. § 102(a) be withdrawn.

Claim 57 is not anticipated by Beger et al. for at least the reasons given for claim 18. In addition, Beger et al. does not teach or suggest calculated nuclear magnetic resonance data as recited in claim 57. Applicants request that the rejection of claim 57 under 35 U.S.C. § 102(a) be withdrawn.

Claim 58 is not anticipated by Beger et al. for at least the reasons given for claim 18. In addition, Beger et al. does not teach or suggest calculated ^{13}C NMR data as recited in claim 58. Applicants request that the rejection of claim 58 under 35 U.S.C. § 102(a) be withdrawn.

2. Bursi et al.

Claims 1, 3-9, 14-15, 17, 18-21, 25-26 and 55-58 were rejected for allegedly being anticipated by Bursi et al. (*J. Chem. Inf. Comput. Sci.*, **39**: 861-867, 1999). Applicants traverse this rejection and ask that it be withdrawn.

Applicants agree with the acknowledgement in the Office action that the feature of scaling spectral data prior to deriving a pattern (previously included in claim 10, which was not rejected under 35 U.S.C. § 102) is not taught or suggested by Bursi et al. This feature is now included in claim 1. Claim 1, as amended, recites the feature of "scaling the spectral data of the training set of compounds prior to deriving a pattern associated with the biological activity." Claim 1 is therefore not anticipated by Bursi et al., and applicants request that the rejection of claim 1 be withdrawn.

Claims 3 and 4 are not anticipated by Bursi et al. for at least the reasons given for claim 1. Applicants request that the rejection of claims 3 and 4 under 35 U.S.C. § 102(a) be withdrawn.

Claim 5 is not anticipated by Bursi et al. for at least the reasons given for claim 1. In addition, Bursi et al. does not teach or suggest the feature of obtaining a pattern of spectral data of a test compound by segmenting the spectral data of the test compound into substantially the same sub-spectral units into which the spectral data of the training set is segmented.

Claims 6-9, 14 and 15 are not anticipated by Bursi et al. for at least the reasons given for claim 1. Applicants request that the rejection of claims 6-9, 14 and 15 under 35 U.S.C. § 102(a) be withdrawn.

Claim 17 is not anticipated by Bursi et al. for at least the reasons given for claim 1. In addition, Bursi et al. does not appear to teach or suggest using artificial intelligence pattern recognition as recited in claim 17. Applicants request that the rejection of claim 3 under 35 U.S.C. § 102(a) be withdrawn.

Claim 18 is not anticipated by Bursi et al. because Bursi et al. does not teach or suggest at least the feature of scaling spectral data as recited in Claim 18. Applicants request that the rejection of claim 18 under 35 U.S.C. § 102(a) be withdrawn.

Claims 19-21, 25-26 and 55-58 are not anticipated by Bursi et al. for at least the reasons given for claim 18. Applicants request that the rejection of claims 19-21, 25-26 and 55-58 under 35 U.S.C. § 102(a) be withdrawn.

All claims are in condition for allowance and such action is requested. If any issues remain before a Notice of Allowance is issued, the Examiner is invited to telephone the undersigned attorney at the number given below.

Respectfully submitted,

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Marked-up Version of Amended Specification and ClaimsPursuant to 37 C.F.R. §§ 1.121(b)-(c)

In the Specification

Marked-up version of Paragraph appearing at page 33, lines 2-12

The estrogenic relative binding affinities (RBAs) of the 30 compounds were obtained from previous publications (Kuiper et al., *Endocrinology* **138**:863-870, 1997; and Tong et al., *Endocrinology*, **138**:4022-4025, 1997). Most of the ^{13}C NMR spectrometric and EI mass spectrometric data were obtained from the Integrated Spectral Data Base System for Organic Compounds (AIST, Japan) [web site www.aist.go.jp/RIODB/SDBS], the *Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra* (Pouchert and Behnke, Eds., Aldrich Chemical Company, Volumes 1-3, 1993), *Spectral Data of Steroids* (Frenkel and Marsh, eds., Thermodynamics Research Center: College Station, 1994), and the NIST MS database software version 1.6. Experimental ^{13}C NMR and EI MS data for five compounds were obtained using standard methods.

Marked-up version of paragraph appearing at page 47, lines 9-18

The biodegradation data for many monocyclic chlorobenzene derivatives in sediment may be found in the Database for Environmental Fate of Chemicals (AIST, Japan) [(www.aist.go.jp/RIODB/dbefc)]. Additional data on the biodegradability is published in *Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL,* Japan Chemical Industry Ecology-Toxicology & Information Center (JETOC), Tokyo, Japan, 1992. The half-life period is used as the endpoint for the establishment of the SDAR and compounds are classified into two endpoint classes as readily biodegradable (R) (half-life < 30 days) and not readily biodegradable (NR) (half-life >30 days). The endpoint data for 34 chlorobenzene derivatives are given in Table 3 below.

Marked-up version of paragraph appearing at page 49, lines 1-8

Spectral data for these chlorobenzene compounds is obtained from the Integrated Spectral Data Base System for Organic Compounds (AIST, Japan) [web site, www.aist.go.jp/RIODB/SDBS], the *Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra* (Poucher and Behnke, Eds., Aldrich Chemical Company, Volumes 1-3, 1993) and the NIST MS database software version 1.6. Experimental ^{13}C NMR, EI MS, and IR data is collected when spectral

data is not available in a database. Experimental spectral data is collected using standard spectroscopic protocols.

Marked-up version of paragraph appearing at page 51, lines 20-28

Phototosensitized oxidations involving singlet oxygen, a strong oxidant, are implicated in photodynamic inactivation of viruses and cells, in phototherapy for cancer, in photocarcinogenesis and in photodegradation of dyes and polymers. Quenching of excited singlet and triplet states of many substances by ground state molecular oxygen produces singlet oxygen; the lowest electronically excited singlet state of molecular oxygen. A compilation of the quantum yields for the formation of singlet oxygen in fluid solutions for over 700 substances is available from the Notre Dame Radiation Laboratory – Radiation Chemistry Data Center. [(http://www.rcdc.nd.edu).]

Marked-up version of paragraph appearing at page 56, lines 1-8:

For each of the structures generated using the combinatorial chemistry software, ^{13}C NMR spectra are predicted. The ^{13}C NMR spectra may be predicted by any known method. Examples of methods for predicting ^{13}C NMR spectra include the neural network methods described by Kvasnicka (Kvasnicka, V., *J. Math. Chem.*, **6**: 63-76, 1991) and the quantum mechanical calculations of Dios et al. (Dios et al., *Science* **260**:1491-1496, 1993). Software for predicting ^{13}C NMR spectra is also available from Advanced Chemistry Development, Toronto, Ontario, Canada [(www.acdlabs.com)] (ACD/CNMR Spectrum Generator).

Marked-up version of paragraph appearing at page 63, lines 3-10

In another embodiment of the invention, ^{13}C NMR spectral data are predicted by calculation (see, for example, Dios et al., *Science* **260**:1491-1496, 1993 and Kvasnicka, V., *J. Math. Chem.*, **6**: 63-76, 1991) and used in an SDAR model that has been trained on true ^{13}C NMR spectral data. Software for predicting ^{13}C NMR spectra is also available from Advanced Chemistry Development, Toronto, Ontario, Canada [(www.acdlabs.com)] (ACD/CNMR Spectrum Generator). Predicted ^{13}C NMR spectral data may be used, for example, to aid in rational drug design by allowing proposed structures to be tested for potential activities before synthesis is attempted.

Marked-up version of paragraph appearing at page 66, lines 15-23

Statistical methods include Principal Component Analysis (PCA) and variations of PCA such as linear regression analysis, cluster analysis, canonical variates, and discriminant analysis, soft independent models of class analogy (SIMCA), expert systems, and auto spin (see, for example, Harrington, *RESolve Software Manual*, Colorado School of Mines, 1988, incorporated by reference). Other examples of statistical analysis software available for principal-component-based methods include SPSS (SPSS Inc., Chicago, IL), JMP (SAS Inc., Cary NC), Stata (Stata Inc., College Station, TX) and Cluster[(available to run from entropy:~dblank/public_html/cluster)].

In the Claims

1. (Amended) A method of predicting a biological activity of a test compound [molecule], comprising:

obtaining spectral data for the [a] test compound and for a training set of compounds having known biological activities;

scaling the spectral data of the training set of compounds prior to deriving a pattern of spectral data associated with the biological activity;

[comparing the spectral data of the test compound to] deriving [a] the pattern of spectral data associated with the [a] biological activity[, derived not exclusively] from the [assigned] spectral data of a training set of compounds [having a known biological activity]; and

predicting the biological activity of the test compound by detecting similarities between the pattern of spectral data associated with [a] the biological activity [of the training set] and a pattern of spectral data for the test compound. [to determine whether the test compound is predicted to share the biological activity.]

2. (Amended) The method of claim 1, wherein the spectral data are obtained without first correlating the spectral data with corresponding structural features.

3. (Amended) The method of claim 1, wherein the pattern of spectral data associated with a biological activity is derived without first correlating the spectral data with corresponding structural features.

4. (Amended) The method of claim 1, wherein the pattern of spectral data of the training set is a pattern obtained by segmenting [separating] the spectral data of the training set of compounds into sub-spectral units.

5. (Amended) The method of claim 4, wherein the pattern of spectral data of the test compound is obtained by segmenting [separating] the spectral data of the test compound into substantially the same sub-spectral units into which the spectral data of the training set is segmented [separated].

6. (Reiterated) The method of claim 1, wherein the spectral data is one type of spectral data.

7. (Amended) The method of claim 6, wherein the spectral data is [comprises one of] nuclear magnetic resonance, mass spectral, infrared, ultraviolet-visible, fluorescence, or phosphorescence data.

8. (Reiterated) The method of claim 1, wherein the spectral data is a composite of different types of spectral data.

9. (Amended) The method of claim 8, wherein the composite [different types of spectral data] comprises two or more of the group consisting of nuclear magnetic spectroscopy (NMR), mass spectroscopy (MS), infrared (IR) spectroscopy, and ultraviolet-visible (UV-Vis) spectroscopy.

10. (Amended) The method of claim 1, wherein the spectral data of the test compound is segmented into substantially the same sub-spectral units as the spectral data of the training set of compounds to produce the spectral pattern [of] for the test compound. [and the

spectral pattern of the training set are segmented into sub-spectral units, and the spectral data of the training set is scaled to normalize the importance of different signals within the spectral data of the training set prior to deriving a pattern associated with a biological activity.]

11. (Amended) The method of claim 1 [10], wherein [the] scaling comprises [is] auto-scaling.

12. (Amended) The method of claim 1, [10, wherein] further comprising weighting the spectral data of the training set [is weighted] to emphasize signals that are important for determining an [the] endpoint class of compounds in the training set before deriving the [a] pattern associated with the [a] biological activity.

13. (Amended) The method of claim 12, wherein [the] weighting comprises [is] Fisher-weighting.

14. (Amended) The method of claim 1, wherein detecting similarities between the pattern of spectral data associated with a biological activity of the training set and the pattern of spectral data for the test compound comprises statistical [performing computer implemented] pattern recognition.

15. (Amended) The method of claim 10 [1], wherein detecting similarities between the pattern of spectral data associated with a biological activity of the training set and the pattern of spectral data for the test compound comprises detecting relative intensities of [signals associated with] one or more of the sub-units of the pattern of spectral derived from [spectrum of] the training set, and detecting relative intensities of signals associated with the same one or more sub-units of a spectrum of the test compound.

16. (Reiterated) The method of claim 15, wherein the relative intensities are canonical variate factors of the spectral data associated with a biological activity of the training set and the spectral signals of the test compound.

17. (Amended) The method of claim 1, wherein the method [is computer implemented] comprises artificial intelligence pattern recognition.

18. (Amended) A computer implemented method [system] for predicting a biological activity of a test compound, comprising:

receiving [as input] spectral data for a test compound as input;

receiving [as input] spectral data and endpoint data of a training set of compounds having [a] known biological activities as input;[activity; and]

segmenting the spectral data of the training set of compounds into sub-spectral units;

scaling the segmented spectral data of the training set of compounds;

detecting a pattern of spectral data associated with the biological activity; and

predicting the biological activity of the test compound by comparing the pattern of spectral data [of the training set] associated with the biological activity to the spectral [pattern] data of the test compound to determine whether the spectral data [pattern] of the test compound is similar to [matches] the spectral pattern associated with the biological activity of the training set and the test compound is predicted to share the biological activity.

19. (Amended) The computer implemented method [system] of claim 18, wherein comparing [the spectral patterns] comprises comparing with a [the spectral patterns with computer implemented] statistical pattern recognition program[s].

20. (Amended) The computer implemented method [system] of claim 19, wherein the spectral data for the test compound [and the spectral data for the training set are divided] is segmented into substantially identical sub-spectral units as the training set spectral data [bins], so that a signal within an individual sub-spectral unit [bins] is compared to the corresponding sub-spectral unit of the pattern. [compared between spectral patterns of the training set associated with the biological activity and the test compound.]

21. (Amended) The computer implemented method [system] of claim 18, wherein the [spectral patterns are obtained by inputting] spectral data are selected from the group consisting of nuclear magnetic resonance data, mass spectral data, infrared data, ultraviolet-visible

[untraviolet-visible] data, fluorescence data, phosphorescence data, and composites of two or more such spectral data.

22. (Amended) The computer implemented method [system] of claim 21, wherein the [spectral data for the training set are converted into canonical variates] detected pattern associated with the biological activity of the training set is a set of canonical variate factors, and the spectral data for the test compound are compared to the canonical variate[s] factors of the training set spectral data.

23. (Amended) The computer implemented method [system] of claim 22, wherein the biological activity is binding affinity to a hormone receptor, and the canonical variate[s] factors [for the training set] include peaks in sub-spectral units [bins] that are associated with hormone receptor binding of a pre-selected affinity.

24. (Amended) The computer implemented method [system] of claim 23, wherein the spectral data comprise nuclear magnetic resonance data and mass spectral data.

25. (Reiterated) A computer readable medium having stored thereon instructions for performing the actions of claim 1.

26. (Reiterated) A computer readable medium having stored thereon instructions for performing the actions of claim 18.

55. (Amended) The method of claim 1, wherein the spectral data comprises calculated spectral data. [is selected from the group consisting of experimental spectral data, calculated spectral data, and combinations thereof.]

56. (Amended) The computer implemented method [system] of claim 18 [21], wherein the spectral data comprises calculated spectral data. [is selected from the group consisting of experimental spectral data, calculated spectral data, and combinations thereof.]

57. (Amended) The computer implemented method [system] of claim 56, wherein the calculated spectral data comprises [is] calculated nuclear magnetic resonance data.

58. (Amended) The computer implemented method [system] of claim 57, wherein the calculated nuclear magnetic resonance data [spectral data is] comprises calculated ^{13}C NMR data.

65. (Amended) The method of claim 1, further comprising:

predicting a second biological activity of the test compound by comparing the spectral data of the test compound to a second pattern of spectral data associated with the [a] second biological activity to determine if the test compound shares the second biological activity, the second pattern derived using scaled spectral data and known endpoints of a training set of compounds for the second biological activity. [chemical or physical property, derived not exclusively from the assigned spectral data of a training set of compounds having a known chemical or physical property; and

detecting similarities between the pattern of spectral data associated with the chemical or physical property of the training set and a pattern of spectral data for the test compound to determine whether the test compound is predicted to share the chemical or physical property.]